

Review of: "Inhibition Success of a Virtually Created Molecule: Pseudoeriocitrin and Femtomolar Inhibition"

Euzébio Guimarães Barbosa¹

¹ Universidade Federal do Rio Grande do Norte

Potential competing interests: No potential competing interests to declare.

There is a pressing need to validate these findings through rigorous experimental testing, particularly to assess potential toxic effects. The study should thoroughly and explicitly address its limitations, encompassing assumptions made in the computational approach. Employing molecular dynamics simulations, particularly Molecular Mechanics/Poisson-Boltzmann Surface Area (MMPBSA) methods, could offer more robust insights into binding affinity and modes. It is evident that the SWISSADME inputs are inaccurate; therefore, a comprehensive revision of these inputs is imperative for accurate and reliable results.